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L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:51420 CAPLUS
DOCUMENT NUMBER: 136:102232
TITLE: Preparation of 7-substituted tetracycline derivatives for pharmaceutical use as antibacterial agents
INVENTOR(S): Nelson, Mark L.; Frechette, Roger; Viski, Peter; Ismail, Mohamed; Bowser, Todd; Bhatia, Beena; Messersmith, David; McIntyre, Laura; Koza, Darrell; Rennie, Glen; Sheahan, Paul; Hawkins, Paul; Verma, Atul; Warchol, Tad; Bandarage, Upul
PATENT ASSIGNEE(S): Trustees of Tufts College, USA; Paratek Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 97 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004407	A2	20020117	WO 2001-US20766	20010629
WO 2002004407	A3	20020404		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-216760P P 20000707
US 2001-275576P P 20010313
OTHER SOURCE(S): MARPAT 136:102232

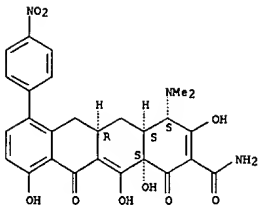
AB 7-Substituted tetracycline derivs., such as I [R7 = NO2, alkyl, alkenyl, alkynyl, aryl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, arylalkyl, amino, arylalkenyl, arylalkynyl, aminoalkyl, etc.], were prepd. for therapeutic use as antibacterial agents. Thus, 7-phenylsancycline I (R7 = Ph) was prepd. in 42% yield by arom. coupling reaction of 7-iodosancycline I (R7 = iodo) with PhB(OH)2 using Pd(OAc)2 and Na2CO3 in MeOH under an argon atm. at r.t. for 2 h. The prepd. tetracycline derivs. were tested for antibacterial activity against Escherichia coli, Enterococcus hirae, and Staphylococcus aureus.

IT **263761-01-9P 389624-24-2P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

RN 263761-01-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

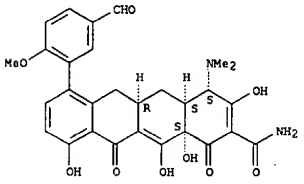
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-24-2 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(5-formyl-2-methoxyphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **263760-96-9P 263760-98-1P 263760-99-2P**
263761-02-0P 380435-62-1P 380435-63-2P
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389624-12-8P 389624-13-9P 389624-21-9P
389624-22-0P 389624-23-1P 389624-28-6P
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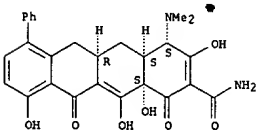
389624-94-6P 389624-97-9P 389624-98-0P
389624-99-1P 389625-02-9P 389625-05-2P
389625-07-4P 389625-08-5P 389625-09-6P

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)
389625-10-9P 389625-12-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

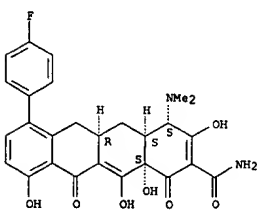
RN 263760-96-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-phenyl-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 263760-98-1 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(4-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

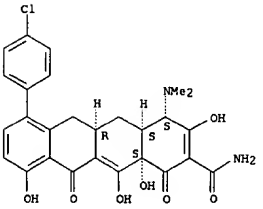
Absolute stereochemistry.



RN 263760-99-2 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(4-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

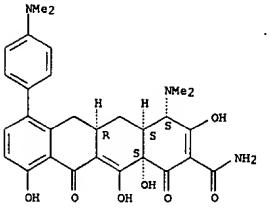
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 263761-02-0 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[4-(dimethylamino)phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

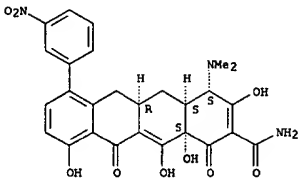
Absolute stereochemistry.



RN 380435-62-1 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(3-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

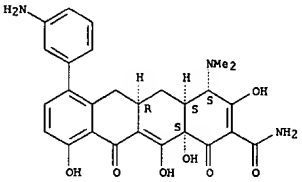
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-63-2 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(3-aminophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

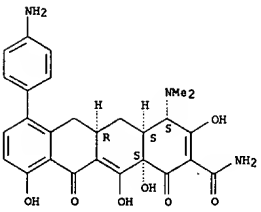
Absolute stereochemistry.



RN 380435-65-4 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(2-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

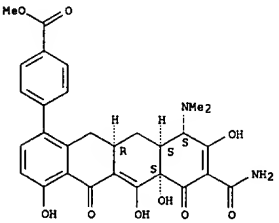
L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



● HCl

RN 389623-72-7 CAPLUS
CN Benzoic acid, 4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-, methyl ester (9CI) (CA INDEX NAME)

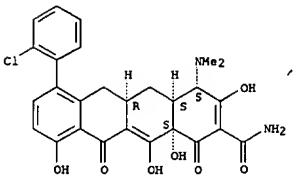
Absolute stereochemistry.



RN 389623-74-9 CAPLUS
CN Benzoic acid, 3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]- (9CI) (CA INDEX NAME)

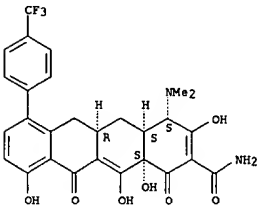
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-76-7 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-(trifluoromethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

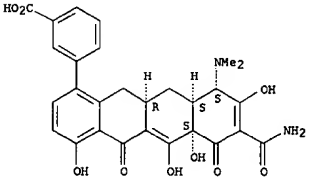
Absolute stereochemistry.



RN 389623-67-0 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(4-aminophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, monohydrochloride, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

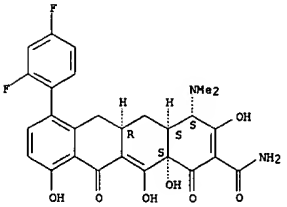
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389623-77-2 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(2,4-difluorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

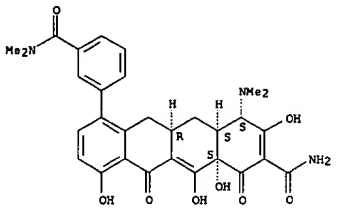
Absolute stereochemistry.



RN 389623-80-7 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[3-[(dimethylamino)carbonyl]phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

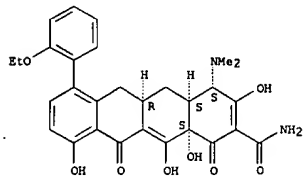
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389623-82-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(2-ethoxyphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

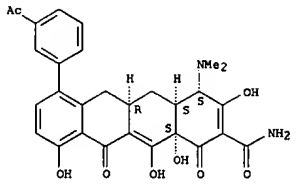
Absolute stereochemistry.



RN 389623-93-2 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(3-acetylphenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

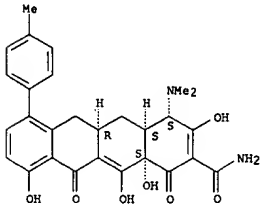
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389623-95-4 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-methylphenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

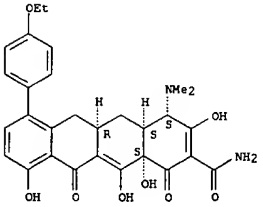
Absolute stereochemistry.



RN 389623-97-6 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(4-ethoxyphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

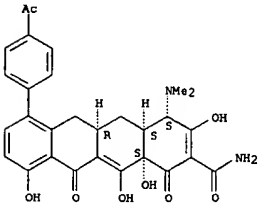
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-03-7 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(4-acetylphenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

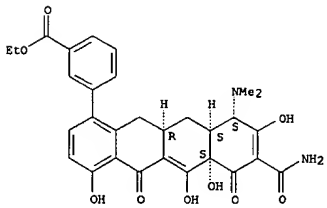
Absolute stereochemistry.



RN 389624-04-8 CAPLUS
CN Benzoic acid, 3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-, ethyl ester (9CI) (CA INDEX NAME)

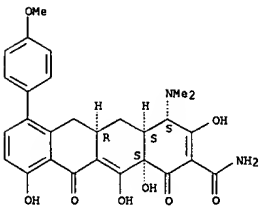
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-05-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-methoxyphenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

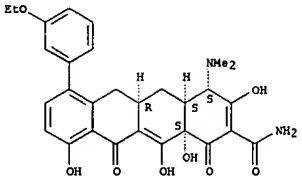
Absolute stereochemistry.



RN 389624-07-1 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(3-ethoxyphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

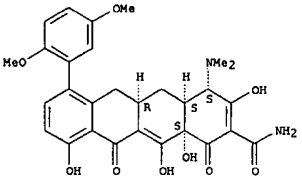
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-12-8 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(2,5-dimethoxyphenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

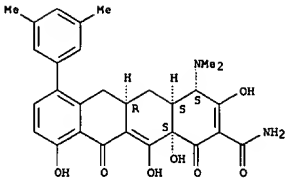
Absolute stereochemistry.



RN 389624-13-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(3,5-dimethylphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

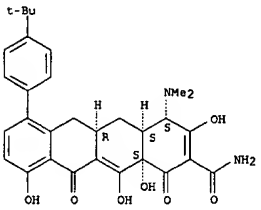
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-21-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[4-(1,1-dimethylethyl)phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

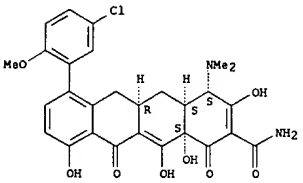
Absolute stereochemistry.



RN 389624-22-0 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(5-chloro-2-methoxyphenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

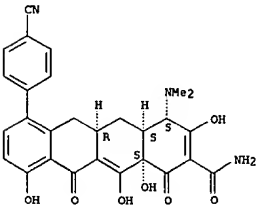
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-23-1 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(4-cyanophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

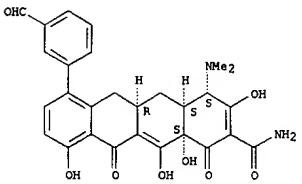
Absolute stereochemistry.



RN 389624-28-6 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(3-formylphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

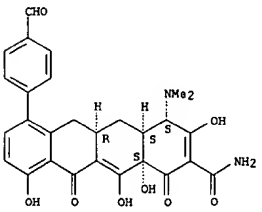
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-29-7 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(4-formylphenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

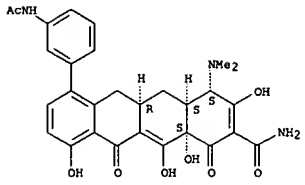
Absolute stereochemistry.



RN 389624-34-4 CAPLUS
CN 2-Naphthacenecarboxamide, 7-[3-(acetylamino)phenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

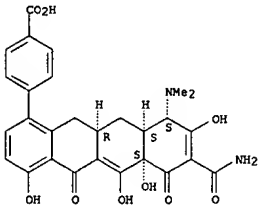
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-45-7 CAPLUS
CN Benzoic acid, 4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]- (9CI) (CA INDEX NAME)

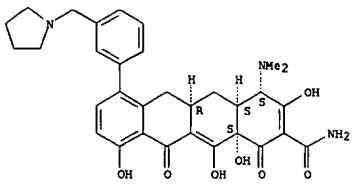
Absolute stereochemistry.



RN 389624-54-8 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[3-(1-pyrrolidinylmethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

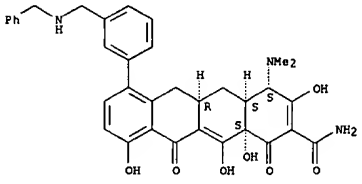
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-55-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[3-[[(phenylmethyl)amino]methyl]phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

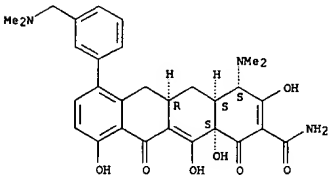
Absolute stereochemistry.



RN 389624-57-1 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[3-[(dimethylamino)methyl]phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

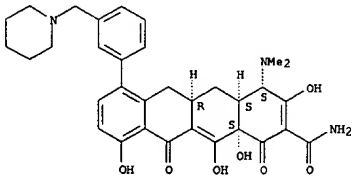
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



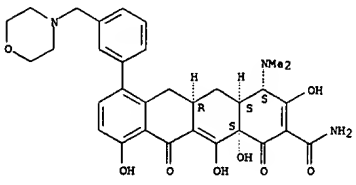
RN 389624-58-2 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[3-(1-piperidinylmethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 389624-59-3 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[3-(4-morpholinylmethyl)phenyl]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

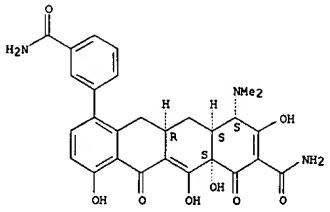
Absolute stereochemistry.



RN 389624-69-5 CAPLUS
CN 2-Naphthacenecarboxamide, 7-[3-(aminocarbonyl)phenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-,

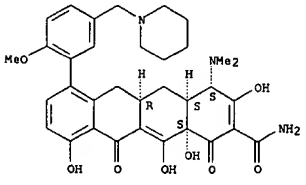
L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)
(4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 389624-81-1 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[2-methoxy-5-(1-piperidinylmethyl)phenyl]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

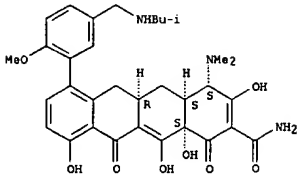
Absolute stereochemistry.



RN 389624-82-2 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[2-methoxy-5-[[(2-methylpropyl)amino]methyl]phenyl]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

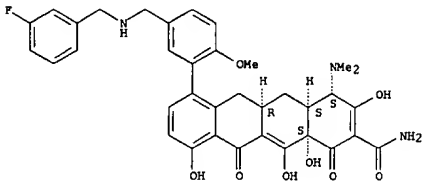
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-90-2 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[5-[[[(3-fluorophenyl)methyl]amino]methyl]-2-methoxyphenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

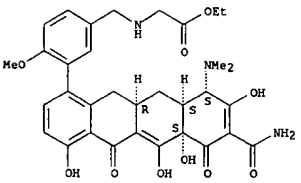
Absolute stereochemistry.



RN 389624-91-3 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[2-methoxy-5-[[(2-phenylethyl)amino]methyl]phenyl]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

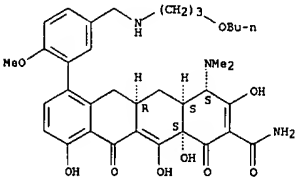
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-94-6 CAPLUS
CN 2-Naphthacenecarboxamide, 7-[5-[[(3-butoxypropyl)amino]methyl]-2-methoxyphenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

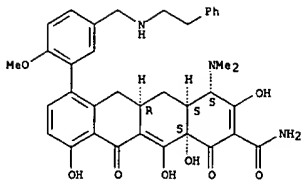
Absolute stereochemistry.



RN 389624-97-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-[[(phenylmethyl)amino]methyl]phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

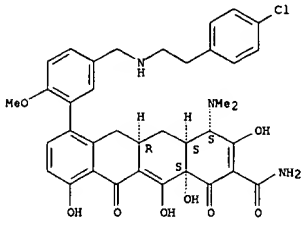
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-92-4 CAPLUS
CN 2-Naphthacenecarboxamide, 7-[5-[[[2-(4-chlorophenyl)ethyl]amino]methyl]-2-methoxyphenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

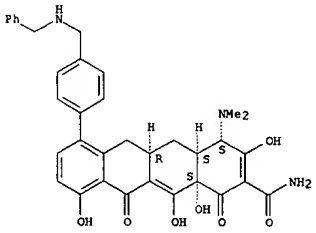
Absolute stereochemistry.



RN 389624-93-5 CAPLUS
CN Glycine, N-[[3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-4-methoxyphenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

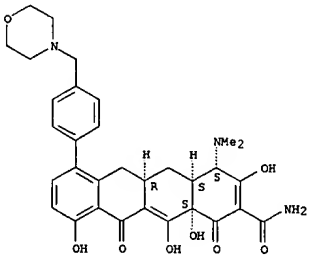
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389624-98-0 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[4-(4-morpholinylmethyl)phenyl]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

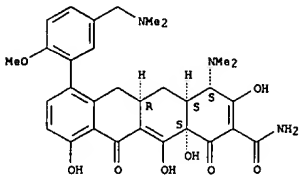
Absolute stereochemistry.



RN 389624-99-1 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[5-[(dimethylamino)methyl]-2-methoxyphenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

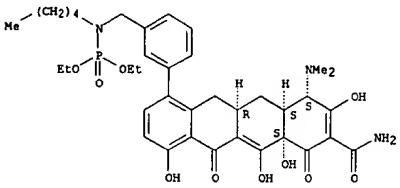
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389625-02-9 CAPLUS
CN Phosphoramidic acid, [[3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]phenyl]methyl]pentyl-, diethyl ester (9CI) (CA INDEX NAME)

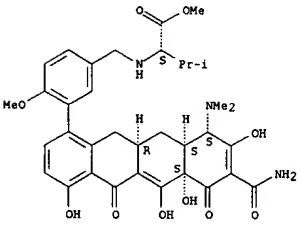
Absolute stereochemistry.



RN 389625-05-2 CAPLUS
CN Benzoic acid, 3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

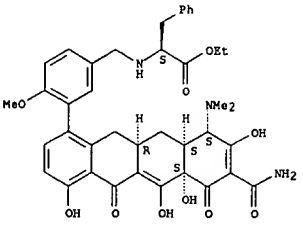
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389625-09-6 CAPLUS
CN L-Phenylalanine, N-[[3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-4-methoxyphenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

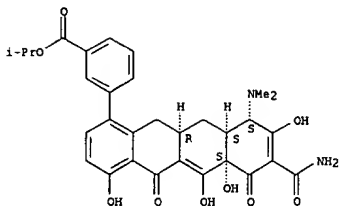
Absolute stereochemistry.



RN 389625-10-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[5-[[[[2-(dimethylamino)ethyl]amino]methyl]-2-methoxyphenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

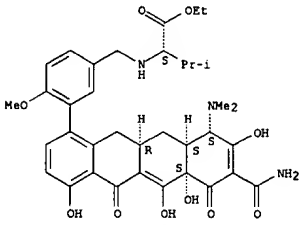
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389625-07-4 CAPLUS
CN L-Valine, N-[[3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-4-methoxyphenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

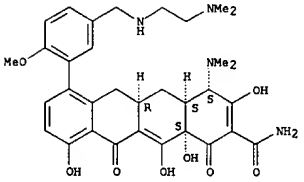
Absolute stereochemistry.



RN 389625-08-5 CAPLUS
CN L-Valine, N-[[3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-4-methoxyphenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

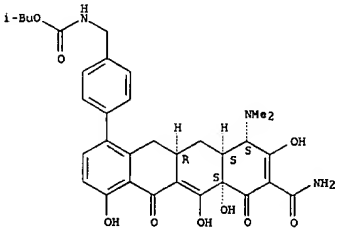
Absolute stereochemistry.

L8 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 389625-12-1 CAPLUS
CN Carbamic acid, [[4-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]phenyl]methyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:51417 CAPLUS
DOCUMENT NUMBER: 136:102229
TITLE: Preparation of 7,8 and 9-substituted tetracycline derivatives
INVENTOR(S): Nelson, Mark L.; Koza, Darrell
PATENT ASSIGNEE(S): Trustees of Tufts College, USA
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004404	A2	20020117	WO 2001-US20558	20010629
WO 2002004404	A3	20020613		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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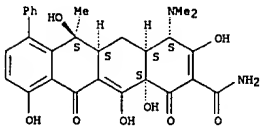
WO 2002012170	A1	20020214	WO 2000-US21366	20000804

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-216656P P 20000707
WO 2000-US21366 W 20000804
OTHER SOURCE(S): MARPAT 136:102229
AB The 7,8 and 9-substituted tetracycline derivs. I (R1 = H, OH; R2, R3 = H, Me, OH; R4 = H, alkenyl, alkynyl, Ph, halophenyl, acyl, phenylalkynyl, heteroaryl, dimethylamino; R5 = H, Ph, nitrophenyl, halo, alkynyl; R6 = H, amino, acetamide, alkynyl; at least one of R4, R5, and R6 is not H) and their pharmaceutically acceptable salts were as antibacterial agents. Thus, tetracycline underwent iodination with NIS to give a mixt. of 7- and 9-iodotetracycline, of which the 7- isomer was treated AsPh3 in presence of Pd(PPh3)2Cl2 and CuI to give 7-phenyltetracycline. I were screened to detn. their in vitro antibacterial min. inhibitory concn. (no data).
IT **389570-44-9P 389570-48-3P 389570-51-8P 389570-52-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 7,8 and 9-substituted tetracycline derivs. as antibacterial agents)
RN 389570-44-9 CAPLUS

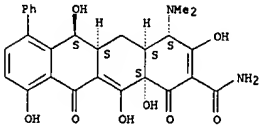
L8 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-7-phenyl-, (4S,4aS,5aS,6S,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



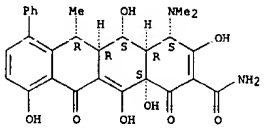
RN 389570-48-3 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-1,11-dioxo-7-phenyl-, (4S,4aS,5aS,6S,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



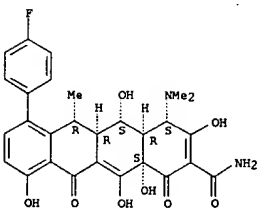
RN 389570-51-8 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-7-phenyl-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 389570-52-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(4-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:935566 CAPLUS
DOCUMENT NUMBER: 136:53633
TITLE: Preparation of 7-phenyl-substituted tetracycline compounds and methods of treating tetracycline responsive states
INVENTOR(S): Nelson, Mark; Rennie, Glen
PATENT ASSIGNEE(S): Trustees of Tufts College, USA
SOURCE: PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

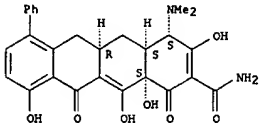
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098259	A1	20011227	WO 2000-US16632	20000616

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-154701P P 19990914
OTHER SOURCE(S): MARPAT 136:53633
AB 7-Phenyl-substituted tetracycline compds., such as I [R4, R4' = alkyl; R5 = H, OH or prodrug moiety; R6, R6' = independently H, OH, alkyl, or taken together, alkenyl; R7 = (substituted)phenyl], and pharmaceutically acceptable salts thereof, are prepd. Thus, 7-phenylsancycline I (R4, R4' = Me; R5, R6, R6' = H; R7 = Ph) was produced from sancycline I (R4, R4' = Me; R5, R6, R6', R7 = H) through iodination at the 7-position with N-iodosuccinimide followed by palladium catalyzed coupling with phenylboronic acid in a combined 42% yield. An in vitro min. inhibitory concn. (MIC) assay used to det. the efficacy of I against common bacteria is described (no data). Addnl., methods of treating tetracycline responsive states, and pharmaceutical compns. contg. the 7-phenyl-substituted tetracycline compds are also described.
IT **263760-96-9P**, 7-Phenylsancycline **263760-98-1P**, 7-(4-Fluorophenyl)sancycline **263760-99-2P**, 7-(4-Chlorophenyl)sancycline **330627-26-4P**, 7,9-Diphenylsancycline **380435-64-3P**, 7-(2-Fluorophenyl)sancycline **380435-65-4P**, 7-(2-Chlorophenyl)sancycline **380435-66-5P**, 7-(2-Bromophenyl)sancycline **380435-67-6P**, 7-(2-Iodophenyl)sancycline **380435-68-7P**, 7-(3-Fluorophenyl)sancycline **380435-69-8P**, 7-(3-Chlorophenyl)sancycline **380435-70-1P**, 7-(3-Bromophenyl)sancycline **380435-72-3P**, 7-(3-Iodophenyl)sancycline **380435-73-4P**, 7-(4-Bromophenyl)sancycline **380435-74-5P**, 7-(4-Iodophenyl)sancycline **380435-75-6P**, 7-(4-Trichloromethylphenyl)sancycline **380435-76-7P**, 7-(4-Trifluoromethylphenyl)sancycline **380435-77-8P**, 7-(4-Tribromomethylphenyl)sancycline **380435-78-9P**, 7-(4-Triiodomethylphenyl)sancycline
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 7-phenyl-substituted tetracycline compds. and methods of treating tetracycline responsive states)

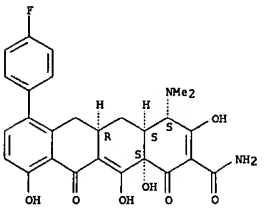
L8 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)
RN 263760-96-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-phenyl-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 263760-98-1 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(4-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



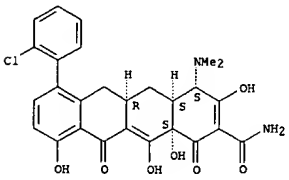
RN 263760-99-2 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(4-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)

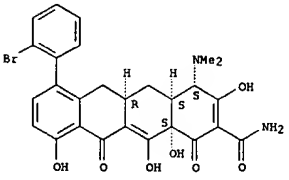
RN 380435-65-4 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(2-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-66-5 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(2-bromophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

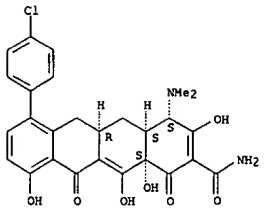
Absolute stereochemistry.



RN 380435-67-6 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(2-iodophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

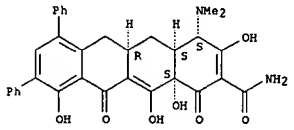
Absolute stereochemistry.

L8 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



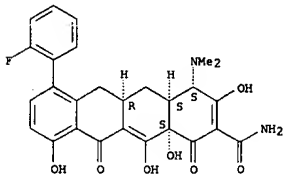
RN 330627-26-4 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7,9-diphenyl-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

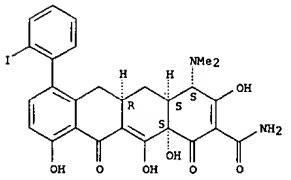


RN 380435-64-3 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(2-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

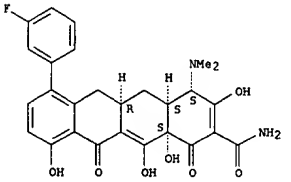


L8 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



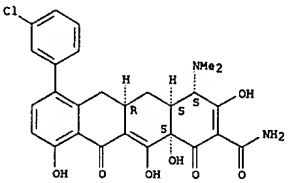
RN 380435-68-7 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(3-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-69-8 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(3-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

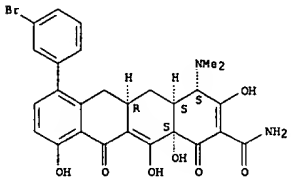
Absolute stereochemistry.



RN 380435-70-1 CAPLUS

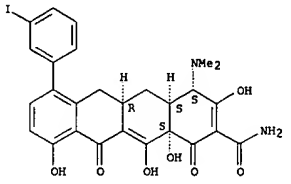
L8 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)
CN 2-Naphthacenecarboxamide, 7-(3-bromophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-72-3 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(3-iodophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

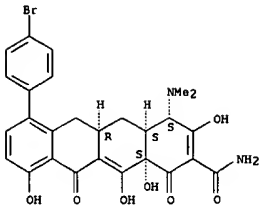
Absolute stereochemistry.



RN 380435-73-4 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(4-bromophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

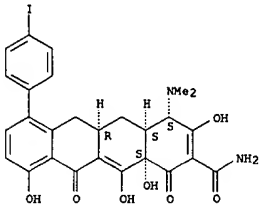
Absolute stereochemistry.

L8 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-74-5 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-iodophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

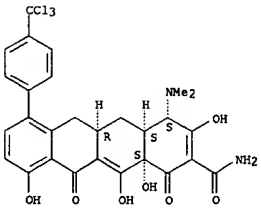
Absolute stereochemistry.



RN 380435-75-6 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-(trichloromethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

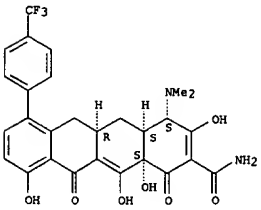
Absolute stereochemistry.

L8 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-76-7 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-(trifluoromethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

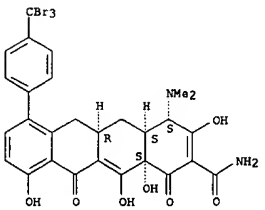
Absolute stereochemistry.



RN 380435-77-8 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-(tribromomethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

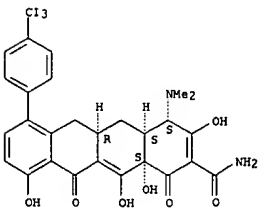
Absolute stereochemistry.

L8 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-78-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-(triiodomethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:935545 CAPLUS
DOCUMENT NUMBER: 136:37446
TITLE: 7-phenyl-substituted tetracycline compds. and methods of treating tetracycline responsive states
INVENTOR(S): Nelson, Mark; Ismail, Mohamed Y.
PATENT ASSIGNEE(S): Trustees of Tufts College, USA
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098236	A2	20011227	WO 2001-US19286	20010615
WO 2001098236	A3	20020328		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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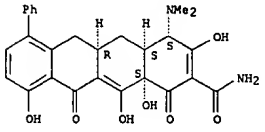
PRIORITY APPLN. INFO.: US 2000-212030P P 20000616
US 2000-212471P P 20000616
OTHER SOURCE(S): MARPAT 136:37446

AB 7-Phenyl-substituted tetracycline compds. of formula I [R1, R2 = alkyl; R3 = H, OH or prodrug moiety; R4, R5 = independently H, OH, alkyl, or, taken together, alkenyl; R6 = (substituted)phenyl] which are substantially free of positional isomers, are prepd. Thus, 7-(3-nitrophenyl)sanclycine (II) was produced from sanclycine through iodination at the 7-position with N-iodosuccinimide followed by palladium catalyzed coupling with 3-nitrophenylboronic acid in a combined 32% yield. An in vitro min. inhibitory concn. (MIC) assay used to det. the efficacy of tetracycline compds. against common bacteria (no data) is described. Addnl., methods of treating tetracycline responsive states, and pharmaceutical compns. contg. the 7-phenyl-substituted tetracycline compds are also described.

IT 263760-96-9P 263760-98-1P 263760-99-2P
263761-02-0P 330627-26-4P 380435-62-1P
380435-63-2P 380435-64-3P 380435-65-4P
380435-66-5P 380435-67-6P 380435-68-7P
380435-69-8P 380435-70-1P 380435-72-3P
380435-73-4P 380435-74-5P 380435-75-6P
380435-76-7P 380435-77-8P 380435-78-9P
380435-79-0P 380435-80-3P 380435-81-4P
380435-82-5P 380435-83-6P 380435-84-7P
380435-85-8P 380435-86-9P 380435-87-0P
380435-88-1P 380435-89-2P 380435-91-6P
380435-92-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(7-phenyl-substituted tetracycline compds. and methods of treating

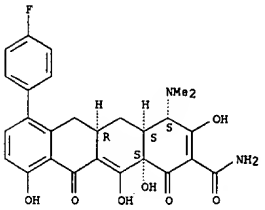
L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)
tetracycline responsive states)
RN 263760-96-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-phenyl-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 263760-98-1 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(4-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

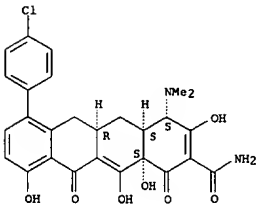
Absolute stereochemistry.



RN 263760-99-2 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(4-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

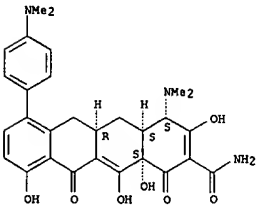
Absolute stereochemistry.

L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



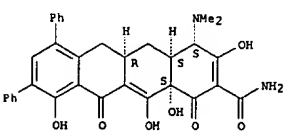
RN 263761-02-0 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[4-(dimethylamino)phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



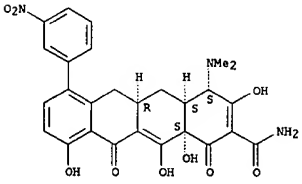
RN 330627-26-4 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7,9-diphenyl-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



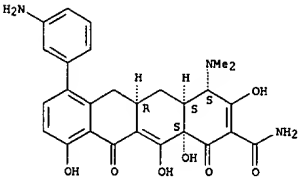
L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)
RN 380435-62-1 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(3-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-63-2 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(3-aminophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

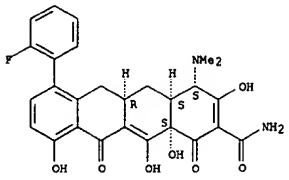
Absolute stereochemistry.



RN 380435-64-3 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(2-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

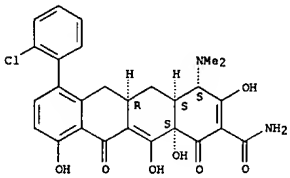
Absolute stereochemistry.

L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



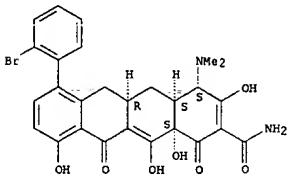
RN 380435-65-4 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(2-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

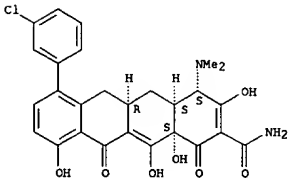


RN 380435-66-5 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(2-bromophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

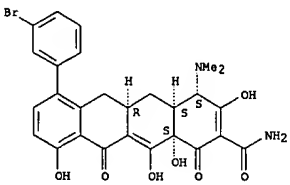


L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



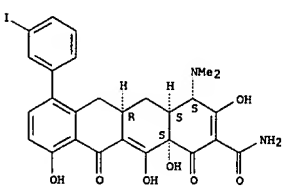
RN 380435-70-1 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(3-bromophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-72-3 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(3-iodophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

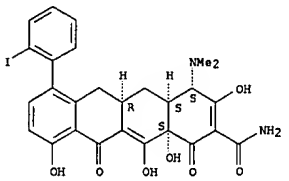
Absolute stereochemistry.



L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)

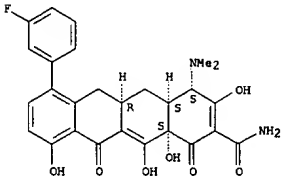
RN 380435-67-6 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(2-iodophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-68-7 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(3-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



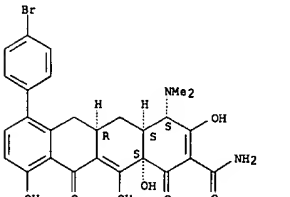
RN 380435-69-8 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(3-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)

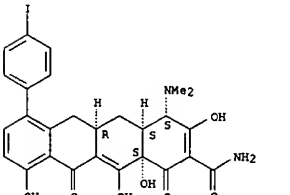
RN 380435-73-4 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(4-bromophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-74-5 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-iodophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

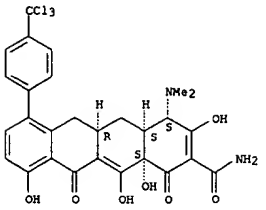
Absolute stereochemistry.



RN 380435-75-6 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-(trichloromethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

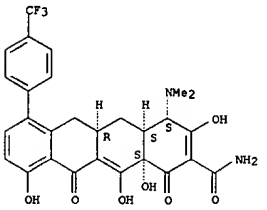
Absolute stereochemistry.

L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-76-7 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-(trifluoromethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

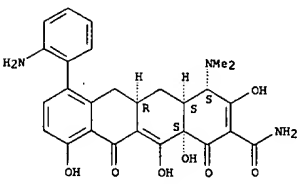
Absolute stereochemistry.



RN 380435-77-8 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-(tribromomethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

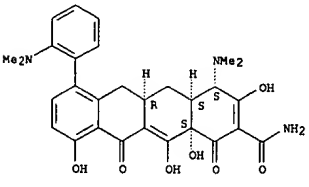
Absolute stereochemistry.

L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



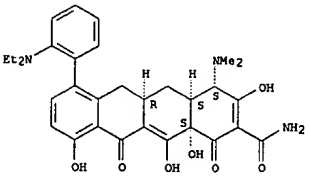
RN 380435-80-3 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[2-(dimethylamino)phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



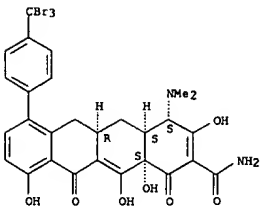
RN 380435-81-4 CAPLUS
CN 2-Naphthacenecarboxamide, 7-[2-(diethylamino)phenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



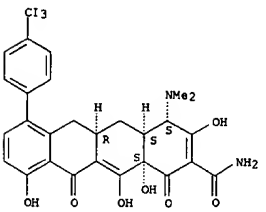
RN 380435-82-5 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[2-(dipropylamino)phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-,

L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-78-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[4-(triiodomethyl)phenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

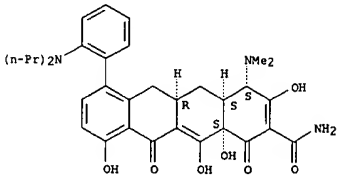


RN 380435-79-0 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(2-aminophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)
(4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-83-6 CAPLUS
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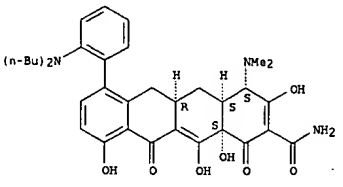
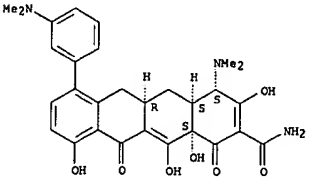
Absolute stereochemistry.



RN 380435-84-7 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[3-(dimethylamino)phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

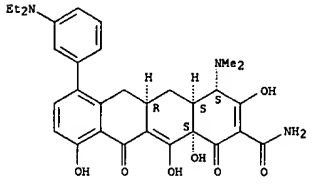
Absolute stereochemistry.



L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)

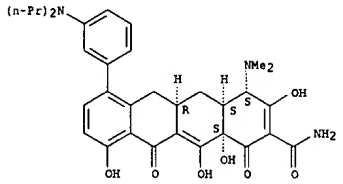
RN 380435-85-8 CAPLUS
CN 2-Naphthacenecarboxamide, 7-[3-(diethylamino)phenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380435-86-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[3-(dipropylamino)phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

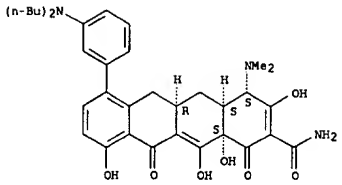
Absolute stereochemistry.



RN 380435-87-0 CAPLUS
CN 2-Naphthacenecarboxamide, 7-[3-(dibutylamino)phenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

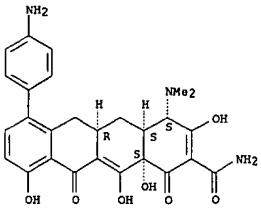
Absolute stereochemistry.

L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-88-1 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(4-aminophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

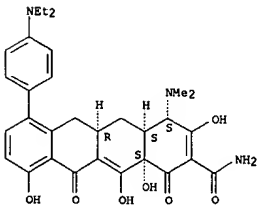
Absolute stereochemistry.



RN 380435-89-2 CAPLUS
CN 2-Naphthacenecarboxamide, 7-[4-(diethylamino)phenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

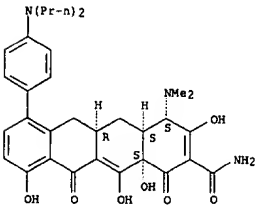
Absolute stereochemistry.

L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380435-91-6 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[4-(dipropylamino)phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

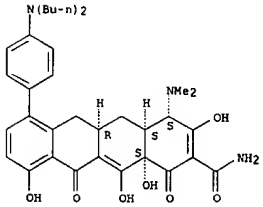
Absolute stereochemistry.



RN 380435-92-7 CAPLUS
CN 2-Naphthacenecarboxamide, 7-[4-(dibutylamino)phenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

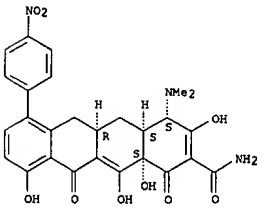
L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



IT **263761-01-9 380435-93-8**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(7-phenyl-substituted tetracycline compds. and methods of treating tetracycline responsive states)

RN 263761-01-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

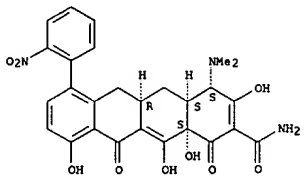
Absolute stereochemistry.



RN 380435-93-8 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(2-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



L8 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:208235 CAPLUS
DOCUMENT NUMBER: 134:252206
TITLE: Methods of preparing substituted tetracyclines with transition metal-based chemistries
INVENTOR(S): Nelson, Mark L.; Rennie, Glen; Koza, Darrell J.
PATENT ASSIGNEE(S): Trustees of Tufts College, USA
SOURCE: PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001019784	A1	20010322	WO 2000-US25040	20000913

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-154701P P 19990914
US 2000-232091P P 20000912
OTHER SOURCE(S): CASREACT 134:252206; MARPAT 134:252206

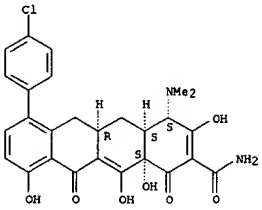
AB Substituted tetracyclinrderivs. were prepd. by combining a reactive tetracycline-based precursor and a reactive org. substituent precursor in the presence of a transition metal catalyst. In one embodiment of the invention, a substituted tetracycline compd. may be prepd. by combining a reactive tetracycline-based precursor compd. such as an arene tetracycline diazonium salt, and a reactive org. substituent precursor, e.g., alkenes, substituted alkenes, vinyl monomers, aroms. and heteroaroms., in the presence of a transition metal catalyst, such as palladium chloride, under conditions such that a tetracycline compd. substituted with the org. substituent is formed. Such compds. may optionally act as intermediates for making other compds., e.g., hydrogenation of unsatd. groups on the substituent. Thus, sancycline-HCl was treated with N-iodosuccinimide in concd. H2SO4 to give 61% 7-iodosancycline and 22% 7,9-diodosancycline. 7-Iodosancycline was added to a degassed soln. of MeOH contg. Na2CO3 and Pd(OAc)2 and then 4-chlorophenylbroonic added to give 7-(4-chlorophenyl)sancycline (I). Antibacterial activity of several derivs. was tabulated.

IT 263760-99-2P 330627-26-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(methods of prepg. substituted tetracyclines with transition metal-based chemistries)

RN 263760-99-2 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(4-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

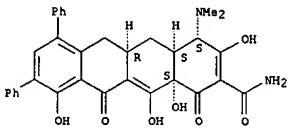
L8 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)

Absolute stereochemistry.



RN 330627-26-4 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7,9-diphenyl-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

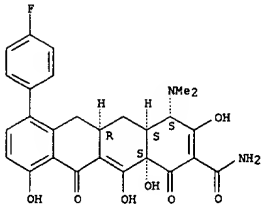


IT 263760-98-1P 263761-01-9P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(methods of prepg. substituted tetracyclines with transition metal-based chemistries)

RN 263760-98-1 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(4-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

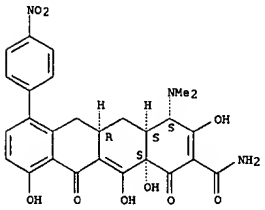
Absolute stereochemistry.

L8 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 263761-01-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

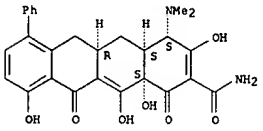
L8 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:137899 CAPLUS
DOCUMENT NUMBER: 132:279036
TITLE: Synthesis of 7-Substituted Tetracycline Derivatives
AUTHOR(S): Koza, Darrell J.
CORPORATE SOURCE: Department of Science and Allied Health, Mount Ida College, Newton, MA, 02459, USA
SOURCE: Organic Letters (2000), 2(6), 815-817
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of 7-substituted tetracycline derivs. has been accomplished in high yield from 7-halotetracyclines by modified Suzuki and Stille coupling protocols. These novel derivs. may serve as a new class of tetracycline antibiotics effective against multi-antibiotic-resistant bacteria.

IT **263760-96-9P 263760-98-1P 263760-99-2P**
263761-01-9P 263761-02-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 7-substituted tetracycline derivs.)

RN 263760-96-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-phenyl-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

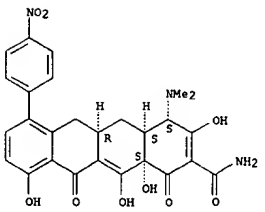
Absolute stereochemistry.



RN 263760-98-1 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(4-fluorophenyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

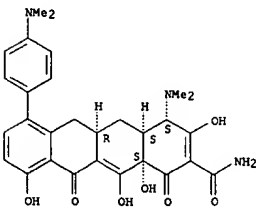
Absolute stereochemistry.

L8 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



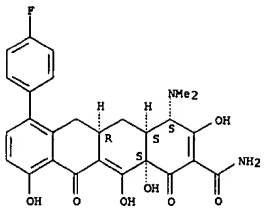
RN 263761-02-0 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[4-(dimethylamino)phenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



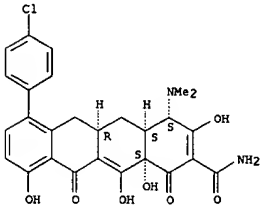
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 263760-99-2 CAPLUS
CN 2-Naphthacenecarboxamide, 7-(4-chlorophenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 263761-01-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-nitrophenyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

=> d ibib ab fqhit 1-5

L10 ANSWER 1 OF 5 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 136:102232 MARPAT
TITLE: Preparation of 7-substituted tetracycline derivatives for pharmaceutical use as antibacterial agents
INVENTOR(S): Nelson, Mark L.; Frechette, Roger; Viski, Peter; Ismail, Mohamed; Bowser, Todd; Bhatia, Beena; Messersmith, David; McIntyre, Laura; Koza, Darrell; Rennie, Glen; Sheahan, Paul; Hawkins, Paul; Verma, Atul; Warchol, Tad; Bandarage, Upul
PATENT ASSIGNEE(S): Trustees of Tufts College, USA; Paratek Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 97 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

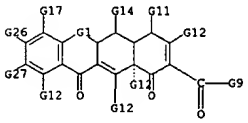
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004407	A2	20020117	WO 2001-US20766	20010629
WO 2002004407	A3	20020404		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-216760P 20000707
US 2001-275576P 20010313

AB 7-Substituted tetracycline derivs., such as I [R7 = NO2, alkyl, alkenyl, alkynyl, aryl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, arylalkyl, amino, arylalkenyl, arylalkynyl, aminoalkyl, etc.], were prepd. for therapeutic use as antibacterial agents. Thus, 7-phenylsancycline I (R7 = Ph) was prepd. in 42% yield by arom. coupling reaction of 7-iodosancycline I (R7 = iodo) with PhB(OH)2 using Pd(OAc)2 and Na2CO3 in MeOH under an argon atm. at r.t. for 2 h. The prepd. tetracycline derivs. were tested for antibacterial activity against Escherichia coli, Enterococcus hirae, and Staphylococcus aureus.

MSTR 1



G1 = 21

L10 ANSWER 1 OF 5 MARPAT COPYRIGHT 2002 ACS (Continued)

G9 = NH2
G10 = Ak<EC (1-) C, BD (0-) D (0-) T> (SO (1-) G6)
G11 = 51

G12 = OH
G17 = Ph (SO (1-) G29)
MPL: claim 1
NTE: and pharmaceutically acceptable salts

L10 ANSWER 2 OF 5 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 136:102229 MARPAT
TITLE: Preparation of 7,8 and 9-substituted tetracycline derivatives
INVENTOR(S): Nelson, Mark L.; Koza, Darrell
PATENT ASSIGNEE(S): Trustees of Tufts College, USA
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004404	A2	20020117	WO 2001-US20558	20010629
WO 2002004404	A3	20020613		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

WO 2002012170	A1	20020214	WO 2000-US21366	20000804

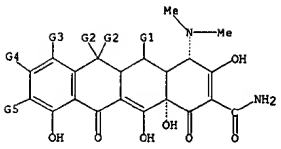
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-216656P 20000707
WO 2000-US21366 20000804

AB The 7,8 and 9-substituted tetracycline derivs. I (R1 = H, OH; R2, R3 = H, Me, OH; R4 = H, alkenyl, alkynyl, Ph, halophenyl, acyl, phenylalkynyl, heteroaryl, dimethylamino; R5 = H, Ph, nitrophenyl, halo, alkynyl; R6 = H, amino, acetamide, alkynyl; at least one of R4, R5, and R6 is not H) and their pharmaceutically acceptable salts were as antibacterial agents. Thus, tetracycline underwent iodination with NIS to give a mixt. of 7- and 9-iodotetracycline, of which the 7- isomer was treated AsPh3 in presence of Pd(PPh3)2Cl2 and CuI to give 7-phenyltetracycline. I were screened to detn. their in vitro antibacterial min. inhibitory concn. (no data).

MSTR 1

L10 ANSWER 2 OF 5 MARPAT COPYRIGHT 2002 ACS (Continued)



G3 = Ph (SO (1-) G6)
MPL: claim 1
NTE: and pharmaceutically acceptable salts

L10 ANSWER 3 OF 5 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 136:53633 MARPAT
TITLE: Preparation of 7-phenyl-substituted tetracycline compounds and methods of treating tetracycline responsive states
INVENTOR(S): Nelson, Mark; Rennie, Glen
PATENT ASSIGNEE(S): Trustees of Tufts College, USA
SOURCE: PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

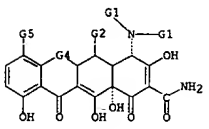
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098259	A1	20011227	WO 2000-US16632	20000616

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-154701P 19990914

AB 7-Phenyl-substituted tetracycline compds., such as I [R4, R4' = alkyl; R5 = H, OH or prodrug moiety; R6, R6' = independently H, OH, alkyl, or taken together, alkenyl; R7 = (substituted)phenyl], and pharmaceutically acceptable salts thereof, are prepd. Thus, 7-phenylsancycline I (R4, R4' = Me; R5, R6, R6', R7 = H) was produced from sancycline I (R4, R4' = Me; R5, R6, R6', R7 = H) through iodination at the 7-position with N-iodosuccinimide followed by palladium catalyzed coupling with phenylboronic acid in a combined 42% yield. An in vitro min. inhibitory concn. (MIC) assay used to det. the efficacy of I against common bacteria is described (no data). Addnl., methods of treating tetracycline responsive states, and pharmaceutical compns. contg. the 7-phenyl-substituted tetracycline compds are also described.

MSTR 1



G1 = Me
G4 = 80

L10 ANSWER 3 OF 5 MARPAT COPYRIGHT 2002 ACS (Continued)

G5 = Ph (SO (1-) G6)
MPL: claim 1
NTE: and pharmaceutically acceptable salts

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 5 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 136:37446 MARPAT
TITLE: 7-phenyl-substituted tetracycline compds. and methods of treating tetracycline responsive states
INVENTOR(S): Nelson, Mark; Ismail, Mohamed Y.
PATENT ASSIGNEE(S): Trustees of Tufts College, USA
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098236	A2	20011227	WO 2001-US19286	20010615
WO 2001098236	A3	20020328		

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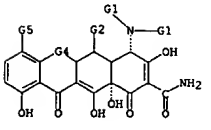
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-212030P 20000616
US 2000-212471P 20000616

AB 7-Phenyl-substituted tetracycline compds. of formula I [R1, R2 = alkyl; R3 = H, OH or prodrug moiety; R4, R5 = independently H, OH, alkyl, or, taken together, alkenyl; R6 = (substituted)phenyl] which are substantially free of positional isomers, are prepd. Thus, 7-(3-nitrophenyl)sanclycine (II) was produced from sanclycine through iodination at the 7-position with N-iodosuccinimide followed by palladium catalyzed coupling with 3-nitrophenylboronic acid in a combined 32% yield. An in vitro min. inhibitory concn. (MIC) assay used to det. the efficacy of tetracycline compds. against common bacteria (no data) is described. Addnl., methods of treating tetracycline responsive states, and pharmaceutical compns. contg. the 7-phenyl-substituted tetracycline compds are also described.

MSTR 1



G1 = Me
G4 = 80

L10 ANSWER 4 OF 5 MARPAT COPYRIGHT 2002 ACS (Continued)

G5 = Ph (SO (1-) G6)
MPL: claim 1
NTE: and pharmaceutically acceptable salts

L10 ANSWER 5 OF 5 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 134:252206 MARPAT
TITLE: Methods of preparing substituted tetracyclines with transition metal-based chemistries
INVENTOR(S): Nelson, Mark L.; Rennie, Glen; Koza, Darrell J.
PATENT ASSIGNEE(S): Trustees of Tufts College, USA
SOURCE: PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001019784	A1	20010322	WO 2000-US25040	20000913
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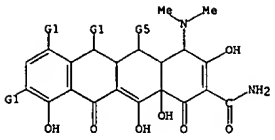
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 1999-154701P 19990914
US 2000-232091P 20000912
OTHER SOURCE(S): CASREACT 134:252206

AB Substituted tetracyclinderivs. were prepd. by combining a reactive tetracycline-based precursor and a reactive org. substituent precursor in the presence of a transition metal catalyst. In one embodiment of the invention, a substituted tetracycline compd. may be prepd. by combining a reactive tetracycline-based precursor compd. such as an arene tetracycline diazonium salt, and a reactive org. substituent precursor, e.g., alkenes, substituted alkenes, vinyl monomers, aroms. and heteroaroms., in the presence of a transition metal catalyst, such as palladium chloride, under conditions such that a tetracycline compd. substituted with the org. substituent is formed. Such compds. may optionally act as intermediates for making other compds., e.g., hydrogenation of unsatd. groups on the substituent. Thus, sancycline-HCl was treated with N-iodosuccinimide in concd. H2SO4 to give 61% 7-iodosancycline and 22% 7,9-diiodosancycline. 7-Iodosancycline was added to a degassed soln. of MeOH contg. Na2CO3 and Pd(OAc)2 and then 4-chlorophenylboronic added to give 7-(4-chlorophenyl)sancycline (I). Antibacterial activity of several derivs. was tabulated.

RN 1

L10 ANSWER 5 OF 5 MARPAT COPYRIGHT 2002 ACS (Continued)



G1 = Ph
MPL: disclosure

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L2            3 S L1
L3           88 S L1 FULL

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L4            1 S L3

     FILE 'REGISTRY' ENTERED AT 14:08:10 ON 06 AUG 2002
L5              STRUCTURE UPLOADED
L6           86 S L5 FULL SUB=L3

     FILE 'USPATFULL' ENTERED AT 14:11:10 ON 06 AUG 2002
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     FILE 'MARPAT' ENTERED AT 14:13:35 ON 06 AUG 2002
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L11           0 S L6

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